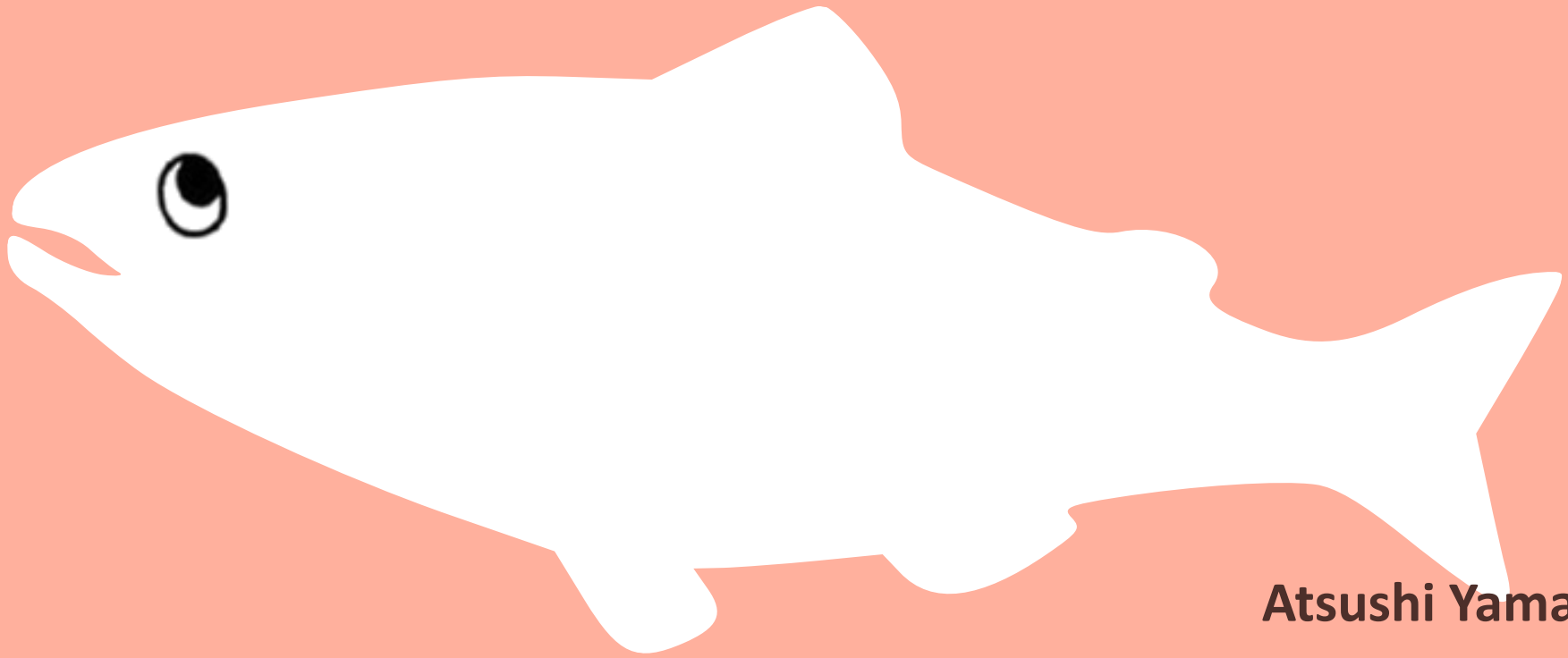
How to Use SALMON: Periodic Systems

Exercise-3



Atsushi Yamada

Center for Computational Sciences, University of Tsukuba

Introduction and Exercise Menu

Option for crystal system (periodic boundary condition):

“iperiodic = 3”

(Input file)

```
....
  sysname = 'Si'
/

&system
  iperiodic = 3
  al = 10.26d0,10.26d0,10.26d0
  isym = 1
  nstate = 32
....
```

Menu of the exercise

Calculations of silicon (Si) :

1. **Ground State**
2. **Dielectric Function**
3. **Real-Time TDDFT Simulation with Incident Laser Pulse**

1. Ground State Calculation (Job Submission)

Prepare files →

```
%> ls
Si_rps.dat  Si_sc_gs.inp
```

Submit job →

```
%> (job submit command)
```

1. Ground State Calculation (input file)

Atomic unit [a.u.] is used as default.
To use Å/fs/eV unit system, give

```
&units
  unit_system='A_eV_fs'
/
```

(but W/cm^2 for electric field (laser) strength)

Si_sc_gs.inp

```
&calculation                    (Calculation Type)
  calc_mode = 'GS'              <- It specifies ground state calculation only
/

&control                        (Control)
  sysname = 'Si'                <- Body name of output file names. e.x. "Si_GS.out"(one of output file names)
/

&system                         (System)
  iperiodic = 3
  al = 10.26d0,10.26d0,10.26d0  <- Unit cell length (cuboid only)
  isym = 1                      <- no symmetry
  nstate = 32                   <- # of bands used in the calculation
  nelec = 32                    <- # of electrons
  nelem = 1                     <- # of atomic species
  natom = 8                     <- # of atoms
/                               (In the case, 16 occupied and 16 unoccupied orbitals are used)

&pseudo                         (Pseudopotential)
  iZatom(1)=14                  <- Atomic number of the 1-th atomic species
  pseudo_file(1) = './Si_rps.dat'  <- File name of pseudopotential
  Lloc_ps(1)=2                  <- Number of the Reference angular momentum (given in the pseudo-potential data file)
/

&functional                     (Functional)
  xc ='BJ_PW'                   <- Functional
/

&rgrid                          (space grid)   (multiples of 4 only)
  num_rgrid = 12,12,12          <- division number of unit cell length
/

&kgrid                          (# of k-points)   (Even number only. User specific k-points is available with reading option of external file)
  num_kgrid = 4,4,4
/

&scf                            (Parameters of Ground State SCF)
  nscf = 120                    <- Maximum iteration number
  threshold=1.0d-7              <- SCF convergence threshold: electron density difference per one electron
/

&atomic_red_coor                (atomic coordinates)
     'Si'   .0    .0    .0     1
     'Si'   .25   .25   .25    1
     'Si'   .5    .0    .5     1
     'Si'   .0    .5    .5     1
     'Si'   .5    .5    .0     1
     'Si'   .75   .25   .75    1
     'Si'   .25   .75   .75    1
     'Si'   .75   .75   .25    1
/
```

[species, x,y,z, species-ID]

Here is reduced coordinate (unit cell length unit).
Use "&atomic_coor" for a.u.(or Å) unit,

1. Ground State Calculation (Output files)

List of Output Files:

- variables.log --- List of inputted variables(keywords) in the calculation
- out.log --- Standard output log

  (Here, this is just example name. The file name is given in your job script file)
- Si_gs_info.data --- Information of GS SCF calculation etc
- Si_k.data --- k-points information
- Si_eigen.data --- Orbital eigen energy values in GS (→ band structure)
- gs_wfn_k/ --- GS wave function

  (This can be used as read-in data in the next calculation)
- PS_Si_KY_n.dat--- Temporary data of pseudopotential
- stdout.log --- Standard output of system (file name given in job.sh)
- stderr.log --- Standard error of system (file name given in job.sh)

1. Ground State Calculation (Check of results)

Followings are useful to check the calculation results.

1. Convergence of SCF calculation (→next page)
   - Standard output (out.log).
   - Si_gs_info.out (this file is generated after SCF finished)
2. Band gap
   - Si_gs_info.out

     Band gaps are printed in the lines of ”Fundamental gap”(indirect transition) and ”BG between same k-point”(direct transition).

1. Ground State Calculation (Check of Convergence of SCF)

```
%> less out.log
```

```
.... (omit) .....
-------------------------------------------
 iter =       62
 Total Energy =  -31.2252432282157     -2.500217455292386E-007
    jav(1),jav(2),jav(3)=   0.551402E-12 -0.197001E-10  0.131539E-10
 (orbital eigen energies)
  1  -0.150535   2  -0.122854   3  -0.122854   4  -0.122854
  5  -0.027750   6  -0.027750   7  -0.027750   8   0.001569
  9   0.129800  10   0.129800  11   0.129800  12   0.151207
 13   0.151207  14   0.151207  15   0.168080  16   0.168080
 17   0.300588  18   0.304820  19   0.304820  20   0.304820
 21   0.338168  22   0.338168  23   0.349556  24   0.349556
 25   0.349556  26   0.360471  27   0.360471  28   0.360471
 29   0.487072  30   0.487079  31   0.487096  32   0.515053
 (forces on atoms)
     1    -0.000000    -0.000000     0.000000
     2    -0.000000    -0.000000    -0.000000
     3     0.000000     0.000000     0.000000
     4    -0.000000     0.000000     0.000000
     5     0.000000     0.000000    -0.000000
     6     0.000000     0.000000    -0.000000
     7    -0.000000    -0.000000    -0.000000
     8     0.000000     0.000000    -0.000000
 e_var_ave,e_var_max=  2.807887450831825E-009  6.335738233753371E-008
 diff-dns,ddns/nelec=  1.019596987160528E-007  7.949054588372419E-008
 -----------------------------------------------
 GS converged at  62
.... (omit) .....
```

Iteration number

Total energy, total energy difference from the last step

Eigen orbital energy of the first k-point

Forces on each atom

Average and Maximum of Eigen energy difference

Total electron density difference (square root of diff.),
Electron density difference per one electron
(absolute value of the diff.)

(The red one is used to judge convergence by default)

Convergence

(Information of GS convergence is also printed in Si_GS.out after the SCF finished)

2. Calculation of Dielectric Function (Job Submission)

Prepare files →

```
%> ls
Si_rps.dat  Si_sc_dielec.inp
```

Copy the pre-calculated → ground state data (or link)

```
%> cp -r (directory of the step 1)/gs_wfn_k/  ./
```

Submit job →

```
%> (job submit command)
```

2. Calculation of Dielectric Function (Input File)

2.Input file for dielectric function calculation: Si_sc_dielec.inp

```
&calculation
 calc_mode = 'RT'
/

&control
 sysname = 'Si'
/
&system
 iperiodic = 3
 al = 10.26d0,10.26d0,10.26d0
 isym = 1
 nstate = 32
 nelec = 32
 nelem = 1
 natom = 8
/
&pseudo
 iZatom(1)=14
 pseudo_file(1) = './Si_rps.dat'
 Lloc_ps(1)=2
/
```

Real-Time: i.e. RS-TDDFT

```
&functional
 xc ='BJ_PW'
/
&rgrid
 num_rgrid = 12,12,12
/
&kgrid
 num_kgrid = 4,4,4
/

&tgrid
 nt=3000
 dt=0.16
/

&propagation
 propagator='etrs'
/
```

(time grid)

# of time steps

Time step size [a.u.]

(time integration)

Algorithm of time integration

```
&emfield
 ae_shape1 = 'impulse'
 epdir_re1 = 0.,0.,1.
/


&atomic_red_coor
      'Si'   .0     .0     .0     1
      'Si'   .25    .25    .25    1
     ..... (omit) ....
      /
```

(Laser/External field)

Type of Laser (or electric field)

Direction of electric field vector

2. Calculation of Dielectric Function (Output Files)

List of Output Files:

- variables.log ---
- out.log ---

} Same as the example 1 (see example 1)

- Si_rt.data --- vector potential, electric fields, current densities (at each time step)
- Si_rt_energy.data-- energies (every 10 steps)
- Si_lr.data --- data from linear response calculation including dielectric function ε(ω) (in the case of ”impulse” keyword)
- PS_Si_KY_n.dat ---
- stdout.log ---
- stderr.log ---

} Log from system (see example 1)

- sc_performance_20171027_155208.log --- measured calculation time

2. Calculation of Dielectric Function (Check of results)

- Output file format of Si_lr.data
  1: Frequency (or Energy) [au]
  2: Re(σ_x), 3: Re(σ_y), 4: Re(σ_z), 5: Im(σ_x), 6: Im(σ_y), 7: Im(σ_z),
  8: Re(ε_x), 9: Re(ε_y), 10: Re(ε_z), 11: Im(ε_x), 12: Im(ε_y), 13: Im(ε_z)

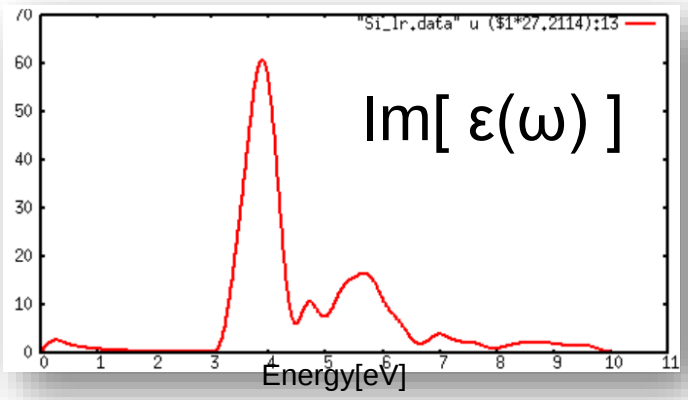
Imaginary part of Dielectric function,
which can be converted to absorption spectrum

```
%> gnuplot
```

```
gnuplot> p "Si_lr.data" u ($1*27.2114):13 w l
```

1au(Hartree)=27.2114eV

→Imaginary part of dielectric function (z-component) as a function of energy



※Tips to get beautiful ε(ω):

- See K.Yabana, et.al., Phys.Rev.B 85,045134 (2012) for the treatment in the small ω.
- Relatively short simulation time (not long simulation time, not very short time) is good to get smooth ε（ω) curve due to the discrete k-points.

3. Real-Time TDDFT Simulation with Incident Laser pulse (Job Submission)

Prepare files →

```
%> ls
Si_rps.dat  Si_sc_pulse.inp
```

Submit job →

```
%> (job submit command)
```

In this calculation, it's not necessary to
copy the pre-calculated ground state data like the previous case
(see the next slide)

3. Real-Time TDDFT Simulation with Incident Laser pulse (Input File)

(Although you can use option to read the ground state wave function as the last example, Altanative option including both of GS calculation & Real-Time TDDFT simulation is used here.)

Input File: Si_sc_pulse.inp

```
&calculation
 calc_mode = 'GS_RT'
/

&control
 sysname = 'Si'
/

&system
 iperiodic = 3
 al = 10.26d0,10.26d0,10.26d0
 isym = 1
 nstate = 32
 nelec = 32
 nelem = 1
 natom = 8
/

&pseudo
 iZatom(1)=14
 pseudo_file(1) = './Si_rps.dat'
 Lloc_ps(1)=2
/
```

GS + RT
(i.e. Ground State calc.
+ Real-Time TDDFT)

```
&functional
 xc ='TBmBJ'
/

&rgrid
 num_rgrid = 12,12,12
/

&kgrid
 num_kgrid = 4,4,4
/

&tgrid
 nt=3000
 dt=0.16
/

&propagation
 propagator='etrs'
/
```

```
&scf
 nscf = 120
 threshold=1.0d-7
/

&emfield
 ae_shape1 = 'Acos2'
 rlaser_int_wcm2_1 = 1d14
 pulse_tw1 = 441.195136248d0
 omega1 = 0.05696145187d0
 epdir_re1 = 0.,0.,1.
/

&atomic_red_coor
      'Si'   .0     .0     .0     1
      'Si'   .25    .25    .25    1
      ..... (omit) .....
/
```

Function Type of Electric Field. Vector potential with $\cos^2$-type envelop

Pulse Intensity at maximum [W/cm^2]

Time width of pulse

Pulse frequency (photon energy)

3. Real-Time TDDFT Simulation with Incident Laser pulse (Input File)

Other analysis options are available.

(→ use &analysis block in input file)

For examples:

- Print DOS → Use keyword like “out_dos=‘y’”
- Print projection analysis → Use keyword like “projection_option=‘gs’”

  (→ number of excited electrons and holes)
- Print electron density (cube format etc) → use keywords like

  out_dns_rt = 'y'

  out_dns_rt_step = 3000

  format3d = 'cube'
- ……

……

3. Real-Time TDDFT Simulation with Incident Laser pulse (Output File)

List of Output Files: (※Other output files can be generated with analysis options in input file)

- variables.log---
- out.log ---

} Same as the example 1,2 (see example 1,2)

- Si_gs_info.data
- Si_eigen.data
- Si_k.data

} Output for ground state calculation (see example 1)

- Si_rt.data
- Si_rt_energy.data
- Si_lr.data

} Output for RT-TDDFT calculation (see example 2)

- PS_Si_KY_n.dat
- stdout.log
- stderr.log

} Log from system (see example 1,2)

- sc_performance_20171027_155208.log

3. Real-Time TDDFT Simulation with Incident Laser pulse (Check of Results)

- Format of output file: Si_rt.data

units are all [a.u.]
c = light speed

1: t
2:$A_x^{ext}(t)$/c, 3:$A_y^{ext}(t)$/c, 4:$A_z^{ext}(t)$/c ← External Vector Potential
5:$E_x^{ext}(t)$ 6:$E_y^{ext}(t)$ 7:$E_z^{ext}(t)$ ← External Electric Field
8:$A_x^{tot}(t)$/c 9:$A_y^{tot}(t)$/c 10:$A_z^{tot}(t)$/c ← Total (External+Induced) Vector Potential
11:$E_x^{tot}(t)$ 12:$E_y^{tot}(t)$ 13:$E_z^{tot}(t)$ ← Total (External+Induced) Electric Field
14:$J_x^m(t)$ 15:$J_y^m(t)$ 16:$J_z^m(t)$ ← Current Density of Matter

- Format of output file: Si_rt_energy.data

1: t 2:$E_{tot}(t)$ 3:$E_{tot}(t) - E_{tot}(0)$
Total Energy Excitation Energy

```
%> gnuplot
```

```
gnuplot> p “Si_rt.data” u 1:7 w l
```
→ Incident Electric Field (z-component)

```
gnuplot> p “Si_rt.data” u 1:16 w l
```
→ Current Density as a function of t (z-component)

```
gnuplot> p “Si_rt_energy.data” u 1:($3*27.2114) w l
```
→ Excitation Energy as a function of time